

# Spin wave theory for antiferromagnetic XXZ spin model on a triangle lattice in the presence of an external magnetic field

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Spin wave theory is applied to a quantum antiferromagnetic XXZ model on a triangle lattice in the presence of an in-plane magnetic field. The effect of the field is found to enhance the quantum fluctuation and to reduce the sublattice magnetization at the intermediate field strength in the anisotropic case. The possible implication to the field driven quantum phase transition from a spin solid to a spin liquid is discussed.

## 1. Introduction

Quantum spin systems in low dimensions continue to be an interesting subject. Quantum fluctuation generally destroys the long range order in one dimension [1], and plays an important role in two dimension [2]. In this paper, we study the ground state of spin- $S$  antiferromagnetic quantum XXZ model on a triangle lattice in the presence of an external in-plane magnetic field.

Our main focus is on the effect of the magnetic field to the quantum fluctuation. It is well known that a spin system becomes polarized at a very high field (above a threshold), which suppresses the quantum fluctuation. It is, however, less clear if the magnetic field enhances or suppresses the quantum fluctuation at intermediate field strength. The latter problem may be important to systems near the boundary of a quantum solid (ordered phase) to quantum liquid (disorder phase) transition. Our interest on this problem is partially motivated by the recent experiments on  $Cs_2CuCl_4$ . That system [3] is a quasi 2-dimensional  $S = 1/2$  frustrated Heisenberg antiferromagnet with a weak anisotropy favoring spins aligned in the basal plane, likely due to the Dzyaloshinskii-Moriya interaction [4]. Coldea et al. [5, 6] have used neutron scattering to study the ground state and the dynamics of the system in high magnetic field. Among the observations, these authors found that the system undergoes phase transitions from a spin solid to a spin liquid to a spin fully polarized states as the in-plane magnetic field increases. Their experiment has raised an interesting theoretical question of the effect of the field on the quantum fluctuation and on the possible field driven quantum spin liquid. The basal plane of  $Cs_2CuCl_4$  consists of a triangle lattice with the spin-spin coupling much stronger along one direction than along other two directions. There have been some theoretical works attempting to address some of the issues relevant to the experiments [7, 8, 9]. Here we shall consider a simplified model to study the field effect on the quantum spin fluctuation. For simplicity, in our model we shall neglect the lattice anisotropy in the real systems, and assume the spin couplings are the same between all the pairs of the nearest neighboring sites. We shall use XXZ model to describe

the anisotropy in spin space, which distinguishes the in-plane field from the perpendicular field.

We apply spin-wave theory [10] to study the leading order correction to the sublattice magnetization due to the quantum fluctuation. The spin wave theory or equivalent theories have been applied to a number of systems, including the antiferromagnetic Heisenberg model in a triangle lattice [11] and the quantum XY model [12]. We calculate the ground state energy and the sublattice magnetization as functions of the magnetic field, and find that the quantum fluctuation measured by the reduction of the sublattice magnetization is enhanced as the field increases at the intermediate field strength and in the anisotropic case. The possible implication to the field driven quantum phase transition will be discussed.

This paper is organized as follows. In section 2, we introduce the model Hamiltonian. Section 3 describes the application of the spin wave theory to the present model. The results for the ground state energy and the sublattice magnetization are presented in section 4. In the final section, we summarize our results and discuss their possible implications to the field driven quantum spin liquid.

## 2. Model Hamiltonian

We consider spin- $S$  antiferromagnetic XXZ model on a triangular lattice of  $3N$  sites in the x-z plane in the presence of an external magnetic field  $h$  along the z-axis. The lattice constant is set to be 1. The Hamiltonian can be written as follows:

$$H = \sum_{i,\delta} (S_i^x S_{i+\delta}^x + S_i^z S_{i+\delta}^z + w S_i^y S_{i+\delta}^y) - Sh \sum_i S_i^z. \quad (1)$$

In the above equation,  $S_i^\mu$  is the  $\mu$  component of the spin- $S$  operator on site  $i$ , and  $\delta$  denotes the three nearest-neighbor bond vectors (see Fig.1) given by,  $\delta_\alpha = (1, 0)$ ,  $\delta_\beta = (-1/2, \sqrt{3}/2)$ , and  $\delta_\gamma = (-1/2, -\sqrt{3}/2)$ .  $hS$  is the strength of the magnetic field, and  $h$  will be considered to be order of unity for the purpose of analyzing the spin wave theory, so that the magnetic field contribution to

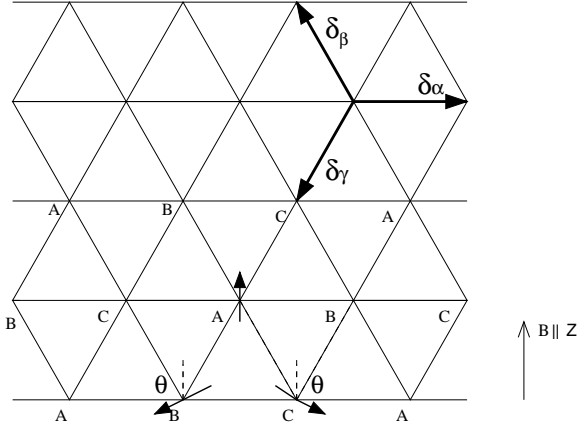


FIG. 1: Three sublattices in a triangle lattice and the classical spin state studied in this paper.

the energy is of the same order as the leading order spin-spin interaction energy.  $w$  is a parameter describing the anisotropy of the model, and  $0 \leq w \leq 1$ . The model is reduced to the Heisenberg model at  $w = 1$ , and to the XY model at  $w = 0$ . Note that the model with  $w > 1$  belongs to a different universal class and will not be discussed here.

### 3. Spin-wave theory

We apply the spin wave theory to study this model [10]. This requires a proper choice of the classical state upon which the spin wave represents minimum quantum fluctuations. Since  $w \leq 1$ , we choose quantization axes within the  $x-z$  plane, and consider the spin quantizations in three sublattices as indicated in Fig. 1. Namely, the spins in sublattice A are aligned along the  $z$ -axis and the spins in sublattices B and C are aligned along the  $\theta$  and  $-\theta$  directions respectively, where  $\theta$  is determined variationally. Such a quantization is consistent with the expected three sublattice classical ground state.

We introduce three boson annihilation operators  $a, b, c$  and their corresponding creation operators by means of the Holstein-Primakoff transformation [13] to represent spins on sublattices A, B, and C, respectively. They are given by  $S_i^{z'} = S - n_i$ ,  $S_i^+ = \sqrt{2S - n_i} d_i$ , and  $S_i^- = d_i^\dagger \sqrt{2S - n_i}$ , where  $d = a, b, c$  for the site  $i \in A, B, C$  respectively.  $n_i = d_i^\dagger d_i$ , and  $z'$  is the corresponding spin quantization axis, and  $S_i^\pm = S_i^{x'} \pm i S_i^{y'}$ . We apply the standard spin wave theory and write the Hamiltonian in terms of large  $S$ -expansion. The leading order term is proportional to  $S^2$ , which is the energy of the classical ground state given by

$$E_{cl} = NS^2[6 \cos \theta + 3 \cos 2\theta - h(1 + 2 \cos \theta)]. \quad (2)$$

The angle  $\theta$  is determined variationally by  $dE_{cl}/d\theta = 0$ , from which we find

$$\cos \theta = \begin{cases} (h-3)/6, & h \leq h_c = 9 \\ 1, & h \geq h_c \end{cases} \quad (3)$$

Note that the value of  $\theta$  is independent of the spin anisotropic parameter  $w$  for the  $y$ -component of the spin does not play any role in the classical limit. At zero field, we obtain  $\theta = 120^\circ$ , recovering the well known result. The case of  $\theta = 0$  ( $h \geq h_c$ ) corresponds to the ferromagnetic phase where all the spins are fully polarized along the field direction. We see that as the field increases,  $\theta$  decreases from  $120^\circ$  to 0, and the classical antiferromagnetic ground state is gradually transformed into a ferromagnetic state.

The leading order quantum fluctuation to the classical solution is proportional to  $S$ , and it is given by,

$$H_{FL} = 3S \sum_{\vec{k}} D_{\vec{k}}^\dagger \mathcal{M}_{\vec{k}} D_{\vec{k}} + E_{FL}^0(h), \quad (4)$$

where

$$E_{FL}^0(h) = \begin{cases} -9NS/2, & h \leq h_c \\ -3NS(h/2 - 3), & h \geq h_c \end{cases} \quad (5)$$

In Eq. (4), the sum is over the reduced Brillouin zone, and  $D_{\vec{k}}^\dagger = (A_{\vec{k}}^\dagger, \tilde{A}_{-\vec{k}}^\dagger)$ ,  $A_{\vec{k}}^\dagger = (a_{\vec{k}}^\dagger, b_{\vec{k}}^\dagger, c_{\vec{k}}^\dagger)$ , and  $\tilde{A}$  is the transpose of  $A$ .  $\mathcal{M}$  is a  $6 \times 6$  matrix, and can be written in terms of an identity matrix  $\mathcal{I}$  and the Pauli matrix  $\sigma_x$  as

$$\mathcal{M} = \mathcal{I} \otimes (M_0 + M_+) + \sigma_x \otimes M_- \quad (6)$$

where  $M_0$  is a  $3 \times 3$  diagonal matrix, whose matrix elements are given by  $(M_0)_{11} = \frac{h}{6} - \cos \theta$ , and  $(M_0)_{22} = (M_0)_{33} = \frac{1}{6}(h \cos \theta - 3 \cos \theta - 3 \cos 2\theta)$ , and

$$M_{\pm} = \begin{pmatrix} 0 & (\cos \theta \pm w) \gamma_{\vec{k}} & (\cos \theta \pm w) \gamma_{\vec{k}}^* \\ (\cos \theta \pm w) \gamma_{\vec{k}}^* & 0 & (\cos 2\theta \pm w) \gamma_{\vec{k}} \\ (\cos \theta \pm w) \gamma_{\vec{k}} & (\cos 2\theta \pm w) \gamma_{\vec{k}}^* & 0 \end{pmatrix} \quad (7)$$

In the above equations,  $\gamma_{\vec{k}} = (1/12) \sum_{\delta} \exp(i\vec{k} \cdot \vec{\delta})$ , where the sum of  $\delta$  runs over  $\{\delta_\alpha, \delta_\beta, \delta_\gamma\}$ . The off diagonal matrices  $M_{\pm}$  represents the interaction among the three sublattices. The  $\theta$  term in the matrix elements arises from the  $x$ - and  $z$ - components of the spin fluctuation and the  $w$  term arises from the  $y$ - component of the spin fluctuation.

$H_{FL}$  can be diagonalized by using the Bogoliubov transformation. We introduce three bosonic operators  $\alpha_{n,\vec{k}}$  with  $n = 1, 2, 3$ , and vector operators  $\mathcal{A}_{\vec{k}}^\dagger = (\alpha_{1,\vec{k}}^\dagger, \alpha_{2,\vec{k}}^\dagger, \alpha_{3,\vec{k}}^\dagger)$ . and  $\mathcal{D}_{\vec{k}}^\dagger = (\mathcal{A}_{\vec{k}}^\dagger, \tilde{\mathcal{A}}_{-\vec{k}}^\dagger)$ . They are related to the original Holstein-Primakoff boson operators,

$D_{\vec{k}}$ , by a Bogoliubov transformation  $U$ , and that  $H_{FL}$  is diagonalized in terms of these new boson operators,

$$D_{\vec{k}} = U \mathcal{D}_{\vec{k}} \quad (8)$$

$$H_{FL} = 2S \sum_{n,\vec{k}} \omega_{n,\vec{k}} (\alpha_{n,\vec{k}}^\dagger \alpha_{n,\vec{k}} + 1/2) + E_{FL}^0(h) \quad (9)$$

where  $\omega_{n,\vec{k}}$  ( $n = 1, 2, 3$ ) are the energy dispersions of the three spin wave excitations (magnon modes) in the spin ordered ground state.

In general, the Bogoliubov transformation can be carried out hence the magnon dispersions can be calculated numerically. This will be discussed in the following section. In the ferromagnetic phase,  $h \geq h_c$ , we have analytical results,

$$\omega_{n,\vec{k}} = \sqrt{[-3 + \frac{h}{2} + 3(1+w)T_{n,\vec{k}}]^2 - [3(1-w)T_{n,\vec{k}}]^2}$$

where  $T_{n,\vec{k}} = \gamma_{\vec{k}} \xi^n + \gamma_{\vec{k}}^* \xi^{2n}$ , with  $\xi = \exp(i2\pi/3)$ . Note that  $-1/4 \leq T_{n,\vec{k}} \leq 1/2$ . This result is in agreement with the previous work [14].

#### 4. Results

In this section, we present the results for the ground state energy and the sublattice magnetization of the antiferromagnetic XXZ model obtained from the spin wave theory described in the previous section.

##### 4.1. Ground state energy

In this subsection, we discuss the ground state energy up to the leading order quantum fluctuation, namely to the order of  $S$  in the large  $S$ -expansions. The ground state energy per bond (there are total  $9N$  bonds in the lattice) is given by

$$\epsilon_0 = \epsilon_{cl} + \epsilon_{fl} \quad (10)$$

where  $\epsilon_{cl}$  and  $\epsilon_{fl}$  are the classical and the fluctuation energies, respectively. From Eq. (2),  $\epsilon_{cl}$  is given by,

$$\epsilon_{cl} = \begin{cases} -(\frac{1}{2} + \frac{h^2}{54})S^2, & h \leq h_C \\ (1 - \frac{h}{3})S^2, & h \geq h_C \end{cases} \quad (11)$$

To obtain  $\epsilon_{fl}$ , we include the zero point energy of the bosons in Eq. (9), which leads to

$$\epsilon_{fl} = \begin{cases} (-\frac{1}{2} + \frac{1}{9N} \sum_{n,\vec{k}} \omega_{n,\vec{k}})S, & h \leq h_C \\ (-\frac{h}{6} - 1) + \frac{1}{9N} \sum_{n,\vec{k}} \omega_{n,\vec{k}})S, & h \geq h_C \end{cases} \quad (12)$$

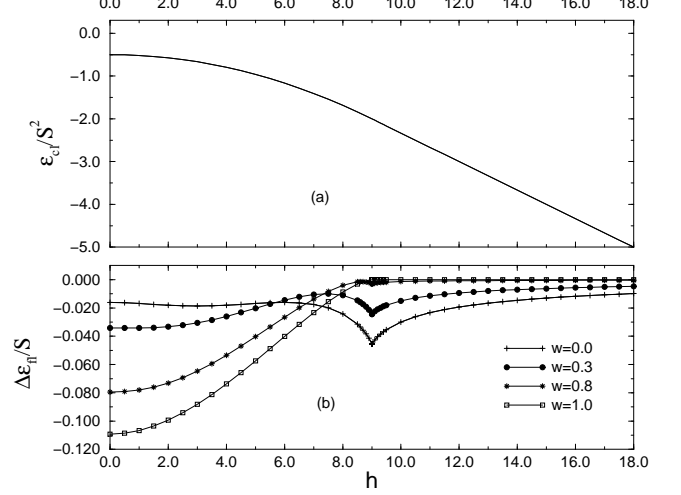


FIG. 2: (a) The classical energy per bond as function of magnetic field  $h$  (b) The leading order quantum correction to the energy in spin wave theory as functions of  $h$  for several values of  $w$ .

We have solved the Bogoliubov transformation problem numerically to diagonalize  $H_{FL}$  and to calculate the dispersions  $\omega_{n,\vec{k}}$  and the energy  $\epsilon_0$ . In Fig. 2(a), we plot the energy of the classical ground state as a function of the magnetic field  $h$ . The energy decreases monotonically as  $h$  increases, and is linear in  $h$  in the ferromagnetic state with  $h \geq h_c$ . In Fig. 2(b), we show the quantum correction to the ground state energy as functions of  $h$  for several values of  $w$ . Firstly, we note that the quantum correction to the energy is very small in comparison with the classical energy even for  $S = 1/2$ . This indicates that the spin wave theory is a good approximation for the present model. At  $h = 0$ , the quantum correction is largest in the Heisenberg model ( $w = 1$ ) and smallest in the XY model ( $w = 0$ ). This is consistent with the intuition that the  $y$ -component of the spin would increase the quantum fluctuation. As  $h$  increases, however, the magnitude of the quantum fluctuation as a function of  $w$  reverses the order as we can see from Fig. 2(b). This becomes apparent at  $h = h_c$ , where the quantum correction to the energy in the Heisenberg model vanishes, while that in the XY model reaches the maximum. It is interesting to note that the magnetic field enhances the quantum fluctuation in certain parameter region of the model, a point we will come back for further discussion in the next subsection. It is also interesting to note that the leading order quantum fluctuation remains finite in the general case even in the ferromagnetic phase. The Heisenberg limit of the model is only a special case where the leading order quantum fluctuation vanishes. The latter can be understood by examining the matrices in  $H_{FL}$ . At  $h \geq h_c$ , and  $w = 1$ , we have  $M_- = 0$ ,

so that boson annihilation operators ( $a, b, c$ ) do not mix with their creation operators ( $a^\dagger, b^\dagger, c^\dagger$ ), hence the system is similar to the ferromagnetic Heisenberg model and has zero quantum fluctuation.

#### 4.2. Sublattice magnetization

We now move to our main interest to discuss the quantum corrections to the sublattice magnetization. The magnetization in sublattice  $L = \{A, B, C\}$  is defined as the average spin component within the same sublattice along its quantization axis,

$$\langle S_L^{z'} \rangle = \frac{1}{N} \sum_{i \in L} \langle S_i^{z'} \rangle = S - \langle \Delta S_L \rangle \quad (13)$$

where  $S$  is the classical value of the spin, and the second term,  $\Delta S_L = (1/N) \sum_{i \in L} \langle d_i^\dagger d_i \rangle$ , is the reduction from the classical spin value due to the quantum fluctuation, and  $\langle Q \rangle$  is the expectation value of operator  $Q$  in the ground state.  $\Delta S_L$  can be calculated from the Bogoliubov transformation matrix  $U$ ,

$$\Delta S_L = \frac{1}{N} \sum_{\vec{k}} |U_{l4}|^2 + |U_{l5}|^2 + |U_{l6}|^2 \quad (14)$$

where  $l = \{1, 2, 3\}$  for  $L = \{A, B, C\}$  respectively, and  $U$  is obtained in the diagonalization of  $H_{FL}$ . The results are shown in Fig. 3 for  $\Delta S_A$  and in Fig. 4 for  $\Delta S_B$  for functions of the field  $h$  for several values of  $w$ . By symmetry,  $\Delta S_C = \Delta S_B$ .

We first discuss the Heisenberg limit of  $w = 1$ . At  $h = 0$ , we find  $\Delta S_L \approx 0.26$  for all the three sublattices. This result is the same as that reported early using a Schwinger boson mean field theory by Yoshioka [11]. As  $h$  increases, both  $\Delta S_A$  and  $\Delta S_B$  decrease, but  $\Delta S_A$  drops much faster as we can see in the figure. For  $h \geq h_C = 9$ , the ground state is ferromagnetic, and we find  $\Delta S_A = \Delta S_B = 0$  as a result of the zero quantum fluctuation in this case as we discussed in the previous subsection.

We now turn to discuss the XY limit of the model with  $w = 0$ . At  $h = 0$ ,  $\Delta S_A = \Delta S_B \approx 0.05$ , which is much smaller than the value in the Heisenberg model ( $\approx 0.26$ ), but is comparable to the value of 0.06 reported in the square lattice XY model [12]. As  $h$  increases from 0,  $\Delta S_A$  decreases to zero while  $\Delta S_B$  increases to reach a maximum at  $h = 3$ . Figs 3 and 4 also show that  $\Delta S_L$  is symmetric with respect to the value of  $h = 3$  in the region  $0 \leq h \leq 6$ . In the XY limit, the quantum fluctuation arising from the  $y$ -component of spin is absent. The off-diagonal matrices  $M_\pm$  in  $H_{FL}$  are given by for  $h \leq h_C$ ,

$$M_\pm = \begin{pmatrix} 0 & \frac{h-3}{6}\gamma_{\vec{k}} & \frac{h-3}{6}\gamma_{\vec{k}}^* \\ \frac{h-3}{6}\gamma_{\vec{k}}^* & 0 & [\frac{(h-3)^2}{18} - 1]\gamma_{\vec{k}} \\ \frac{h-3}{6}\gamma_{\vec{k}} & [\frac{(h-3)^2}{18} - 1]\gamma_{\vec{k}}^* & 0 \end{pmatrix} \quad (15)$$

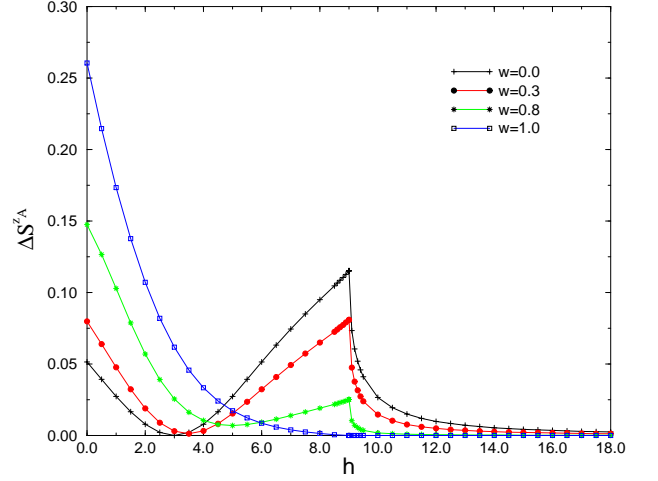


FIG. 3: Quantum correction to local spin in sublattice  $A$  as function of magnetic field  $h$  for several  $w$ .

At  $h = 3$ , there is no finite matrix element between the sublattice  $A$  and sublattices  $B$  or  $C$ . Therefore, the triangle lattice is decomposed into a honeycomb lattice consisting of sublattices  $B$  and  $C$  and  $N$  isolated spins of sublattice  $A$ . Consequently, the spins in  $A$  are all parallel to the field with  $\Delta S_A = 0$ , and  $\Delta S_B$  is the same as the result in a honeycomb lattice in the absence of external fields. The form of  $M_\pm$  also indicate a symmetry with respect to  $h = 3$ , although the rigorous mathematics involves more delicate analyses since the matrices contain elements with both even and odd functions of  $h - 3$ .

As shown clearly in the figures, there are sharp peaks for both  $\Delta S_A$  and  $\Delta S_B$  at  $h = h_c$  except for  $w = 1$ . The peak height increases as  $w$  decreases, and is the largest for  $w = 0$ . Part of this feature found in our calculations may be understood by examining the ferromagnetic phase for  $h \geq h_C$ . In this phase, we have  $\Delta S_A = \Delta S_B = \Delta S$ , which is given by

$$\Delta S = -\frac{1}{2} + \frac{1}{6N} \sum_{n, \vec{k}} \frac{-3 + \frac{h}{2} + 3(1+w)T_{n, \vec{k}}}{\omega_{n, \vec{k}}} \quad (16)$$

From this expression, we see that  $\Delta S$  decreases as  $h$  further increases as we can see from the figures.  $(\partial \Delta S / \partial h)|_{h \rightarrow h_C + 0^+} \rightarrow -\infty$ , so that the slopes of  $\Delta S$  divergent. This explains the singularities of  $\Delta S$  found in our numerical calculation shown in the figures.

The most interesting result we can learn from these calculations is the possible field enhanced quantum fluctuations in certain quantum spin systems. This is somewhat in contrary to the general intuition since the field is expected to partially polarize the spins hence to suppress the quantum fluctuation. Our calculations and analyses demonstrate that this intuitive argument may break

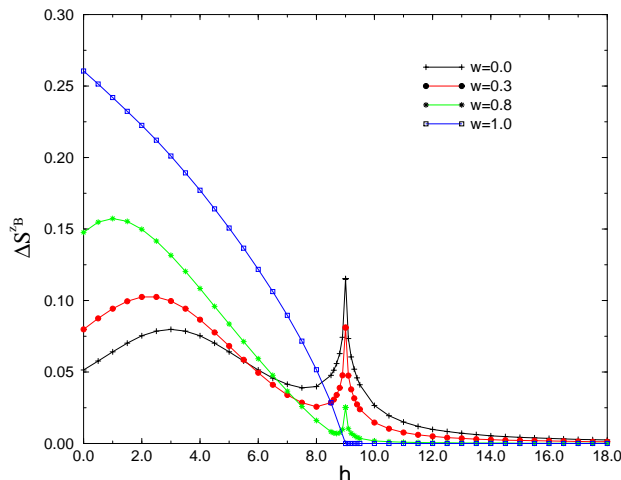


FIG. 4: Same as in Fig. 3 in sublattice B.

down in certain parameter region. This finding should have important implications for the magnetic field driven quantum phase transition from a spin solid to a spin liquid. In the spin wave theory,  $\Delta S$  is a measure of the quantum fluctuation. If  $\Delta S = S$ , the sublattice magnetization vanishes, indicating the melt-down of a quantum solid.

## 5. Discussions and Summary

We have applied the spin wave theory to study quantum XXZ model on a triangle lattice in the presence of an in-plane magnetic field. Our model includes the Heisenberg model at one limit and the XY model at the other limit. We have calculated the ground state energy and the sublattice magnetization as functions of the external field and the anisotropy of the spin coupling. We have found that the field may enhance or suppress the quantum fluctuation and the reduction of the sublattice magnetization, depending on the spin anisotropy and the field strength. At the intermediate field and in the anisotropic case, the field enhances the quantum fluctuation. The reduction of the sublattice magnetization in the model we have studied is still too small to destroy the spin long range order even for the smallest spin system with  $S = 1/2$ . This is because the model we studied here is still quite far from the solid-liquid boundary in the absence of the field. Nevertheless, the qualitative effect of the field on the quantum fluctuation we have found is

interesting, and it may have important implications for systems near the solid-liquid phase boundary. Near that boundary, the external magnetic field may well drive a quantum solid to a quantum liquid due to the increase of the quantum fluctuation. In quasi 2-dimensional triangle lattice of  $Cs_2CuCl_4$ , the in-plane spin-spin couplings are strongly anisotropic, and the coupling along one direction is about three times as large as those along the other two directions. The spin system is between one and two dimensions, and the system in the absence of field has a long range order but is closer to the spin liquid boundary. In that type of systems, an enhanced quantum fluctuation may easily destroy the long range order. We speculate that the in-plane field induced phase transition [6] to the quantum liquid state observed in  $Cs_2CuCl_4$  could be due to the increase of the quantum fluctuation. More detailed calculations on more realistic model would be interesting to carry out to see if such a conjecture is relevant to the experiment.

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